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# 3D simulation of morphological effect on reflectance of $\text{Si}_3\text{N}_4$ sub-wavelength structures for silicon solar cells

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## Abstract

In this study, we investigate the reflectance property of the cylinder, right circular cone, and square pyramid shapes of silicon nitride ( $\text{Si}_3\text{N}_4$ ) subwavelength structure (SWS) with respect to different designing parameters. In terms of three critical factors, the reflectance for physical characteristics of wavelength dependence, the reflected power density for real power reflection applied on solar cell, and the normalized reflectance (reflected power density/incident power density) for real reflectance applied on solar cell, a full three-dimensional finite element simulation is performed and discussed for the aforementioned three morphologies. The result of this study shows that the pyramid shape of SWS possesses the best reflectance property in the optical region from 400 to 1000 nm which is useful for silicon solar cell applications.

## 1. Introduction

Silicon solar cell is one of the promising renewable energy technologies in order to relieve the impact of the climate change. In semiconductor-based solar cells, electron-hole pairs are generated through absorption of impinging photons. Due to high refraction index of semiconductor materials, especially silicon, the incident sunlight power is largely reflected back, resulting in the reduction of light absorption and poor energy conversion efficiency. Antireflection coating (ARC) is mounted over absorption layers, resulting in three effects: (a) reduction in surface reflection, (b) increase in light absorption due to an increase in optical path length by diffraction, and (c) enhancement of internal reflection that reduces the amount of escaping light. Based on the theory of impedance matching, single layer (SLR) and multilayer of ARC are proposed for reduced reflectance property; however, the resulting reflectance spectra meet the demand only within a narrow spectral domain. Sub-wavelength structure's (SWS) dimensions are much smaller than the wavelengths of light; therefore, using ARC on the surface of silicon solar cells can substantially reduce the reflectivity and improve the capability

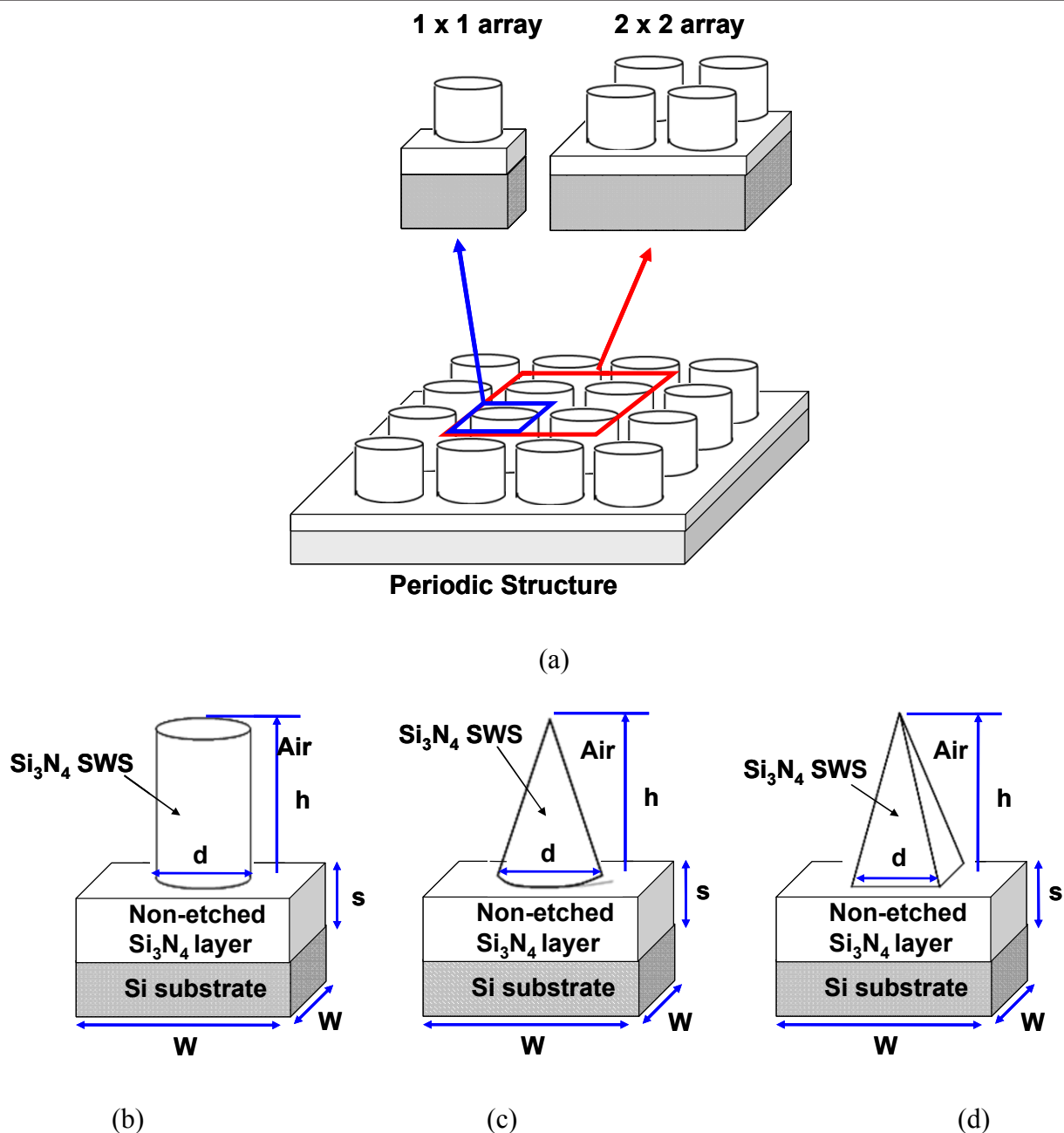
of light trapping. It thus will achieve the enhanced efficiency according to our recent both numerical and experimental studies [1-3]. Compared with silicon solar cell with a SLAR, the efficiency of silicon solar cell with  $\text{Si}_3\text{N}_4$  SWS is promising among various ARC layers in our recent work [4]. A rigorous coupled-wave analysis (RCWA) [1,5-7] has been reported to estimate the reflectance of  $\text{Si}_3\text{N}_4$  SWS by approximating structural shapes with partitioned uniform homogeneous layers. RCWA is an exact solution of Maxwell's equations for the electromagnetic diffraction by grating structures which is generally applicable for 2D plane with 1D periodicity; however, RCWA may suffer numerical difficulties in presence of evanescent orders and it requires a large amount of calculation for retaining several diffraction orders. These factors limit flexible application of RCWA; in particular, for 3D problems with non-azimuthally symmetric structural shapes. Numerical simulation of 3D morphological effect on reflectance property has not been studied yet. Therefore, a full 3D finite-element (FE) analysis of  $\text{Si}_3\text{N}_4$  SWS will be an interesting examination for quantitative understanding of the reflectance property.

In this study, 3D FE simulation for the reflectance of  $\text{Si}_3\text{N}_4$  SWS with three types of structural shapes, the cylinder, the right circular cone, and the square pyramid shapes, is conducted with respect to different geometry

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parameters and lighting angles for quantitative understanding of reflectance property. First, proper selection on the boundary conditions can alleviate the computational load from simulating a holistic ARC. The reflectance of  $\text{Si}_3\text{N}_4$  SWS on the silicon substrate is thus simulated using the 3D finite element method (FEM); consequently, in terms of three critical factors, the reflectance for physical characteristics of wavelength dependence, the reflected power density for real power

reflection applied on solar cell, and the normalized reflectance (reflected power density/incident power density) for real reflectance applied on solar cell are calculated and discussed for the aforementioned three morphologies. The analysis of reflectance spectrum with wide-angle incidences of electromagnetic wave and the average reflectance with various heights are presented. Besides, according to our recent study, which presented the optimal design parameters of  $\text{Si}_3\text{N}_4$  SWS based on



**Figure 1** (a) Plot of the periodic structure of  $\text{Si}_3\text{N}_4$  SWS with  $1 \times 1$  and  $2 \times 2$  arrays as unit cell. 3D schematic plots of the examined (b) cylinder-, (c) right circular cone-, and (d) square pyramid-shaped structure, respectively.

RCWA [4], numerical verification and comparison is accomplished following the discussion. The engineering findings of this study show that the pyramid shape of SWS possesses the best reflectance property in the optical region from 400 to 1000 nm which is useful for silicon solar cell applications.

This rest of the article is organized as follows. In Section 2, we show the computational structure and model. In Section 3, we report the results and discussion. Finally, we draw conclusions and suggest future work.

## 2. The SWS and optical model

Based upon our experimental characterization, Figure 1a illustrates a periodical structure of  $\text{Si}_3\text{N}_4$  SWS which is used in our 3D FE simulation without loss of generality. We study  $\text{Si}_3\text{N}_4$  SWS with the cylinder, the right circular cone, and the square pyramid shapes, as shown in Figure 1b-d, respectively. With a constant volume, the diameter of cylinder- and right circular cone-shaped  $\text{Si}_3\text{N}_4$  SWS and the edge length of square pyramid are 130 nm, the heights (h) of the etched part of  $\text{Si}_3\text{N}_4$  SWS are 200, 600, and 471.3 nm, the height (s) of the non-etched part is 70 nm, and the base (W) of a unit cell is 200 nm [4]. Note that the thickness of Si substrate is given 600 nm. Note that all structural parameters are adopted from our experimental studies [2-4,8]. Throughout the article, we consider time-harmonic fields assuming a time-dependence in  $e^{-j\omega t}$ . The diffraction problem is governed by the well-known Maxwell equations

$$\nabla \times \vec{E} = -j\omega\mu\vec{H}, \quad (1)$$

$$\nabla \times \vec{H} = \vec{J} + j\omega\epsilon\vec{E}, \quad (2)$$

$$\nabla \cdot \vec{E} = \rho/\epsilon, \quad (3)$$

and

$$\nabla \cdot \vec{B} = 0, \quad (4)$$

where  $E$  and  $D$  are electric field intensity and flux density,  $H$  and  $B$  are magnetic field intensity and flux density,  $\lambda$  is the corresponding frequency to the wavelength  $\lambda$ ,  $J$ , and  $\rho$  are current density and charge density,  $\epsilon$  is electric permittivity,  $\mu$  is magnetic permeability. A repeated pattern is applicable to use periodic boundary conditions, thus the Floquet theorem is adopted to simulate the boundary condition of periodic structure. Floquet theorem asserts that the analysis region can be reduced significantly in one periodicity cell to characterize the propagation property. The electric fields in periodic structure are related as follows:

$$\vec{E}_2(\vec{r}) = \vec{E}_1(\vec{r} + \vec{L}) = \vec{E}_1(\vec{r}) e^{-j\theta}, \quad (5)$$

where  $r$  is position vector,  $L$  is the distance between the periodic boundaries, and  $\theta$  is a phase factor determined by wave vector  $k$  and  $L$ :

$$\theta = \vec{k} \cdot \vec{L}, \quad (6)$$

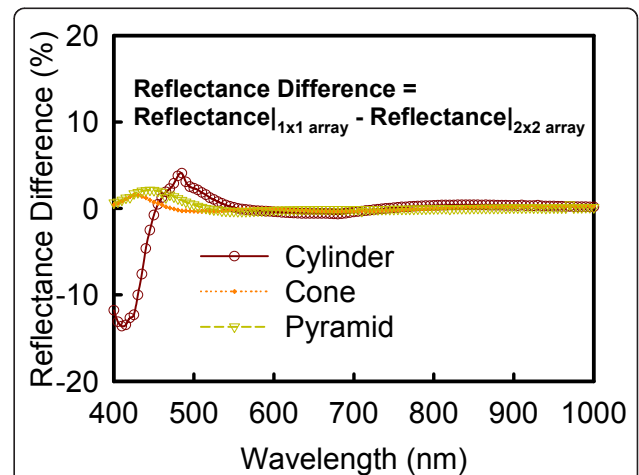
The polarization of transverse electric (TE) mode, in which the electric field is normal to the direction of wave propagation, is excited as the normal incident light source with wavelengths sweeping from 400 to 1000 nm. The bottom region of Si substrate is assigned as perfect matched layer in avoidance of reflected wave. The refraction index of  $\text{Si}_3\text{N}_4$  is 2.05, and the refraction index of Si is frequency dependent with the relation [1]:

$$n_{\text{Si}} = \sqrt{\epsilon + \frac{A}{\lambda^2} + \frac{B\lambda_1^2}{(\lambda^2 - \lambda_1^2)}}, \quad (7)$$

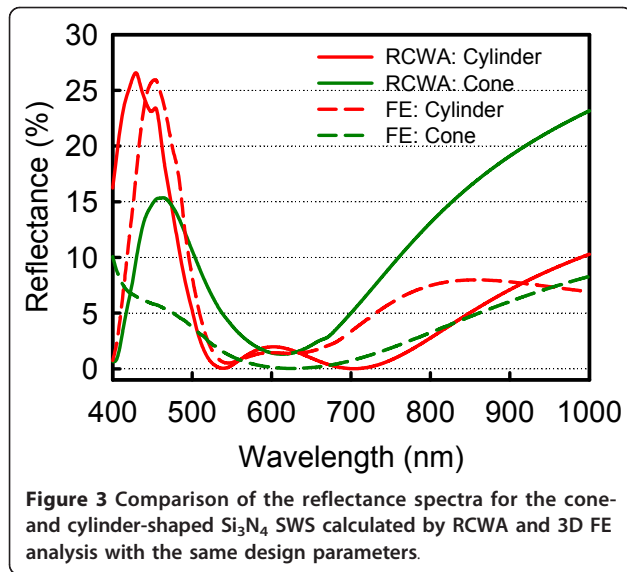
where  $\lambda$  is the incident wavelength,  $A = 0.939816$ ,  $B = 8.10461 \times 10^{-3}$ ,  $\lambda_1 = 1.1071 \mu\text{m}$ , and  $\epsilon = 11.6858$ . The calculation settings of reflectance were reported and can be found in our recent studies [1,4].

## 3. Results and discussion

In order to examine the effect of Floquet boundary condition in 3D FE analysis, as shown in Figure 2, we compare the difference between the simulated unit cells of  $1 \times 1$  and  $2 \times 2$  array of  $\text{Si}_3\text{N}_4$  SWS. We find at the wavelengths above 600 nm, the reflectance of  $1 \times 1$  array of  $\text{Si}_3\text{N}_4$  SWS as unit cell is almost consistent with unit cell of  $2 \times 2$  array, meanwhile insignificant discrepancy

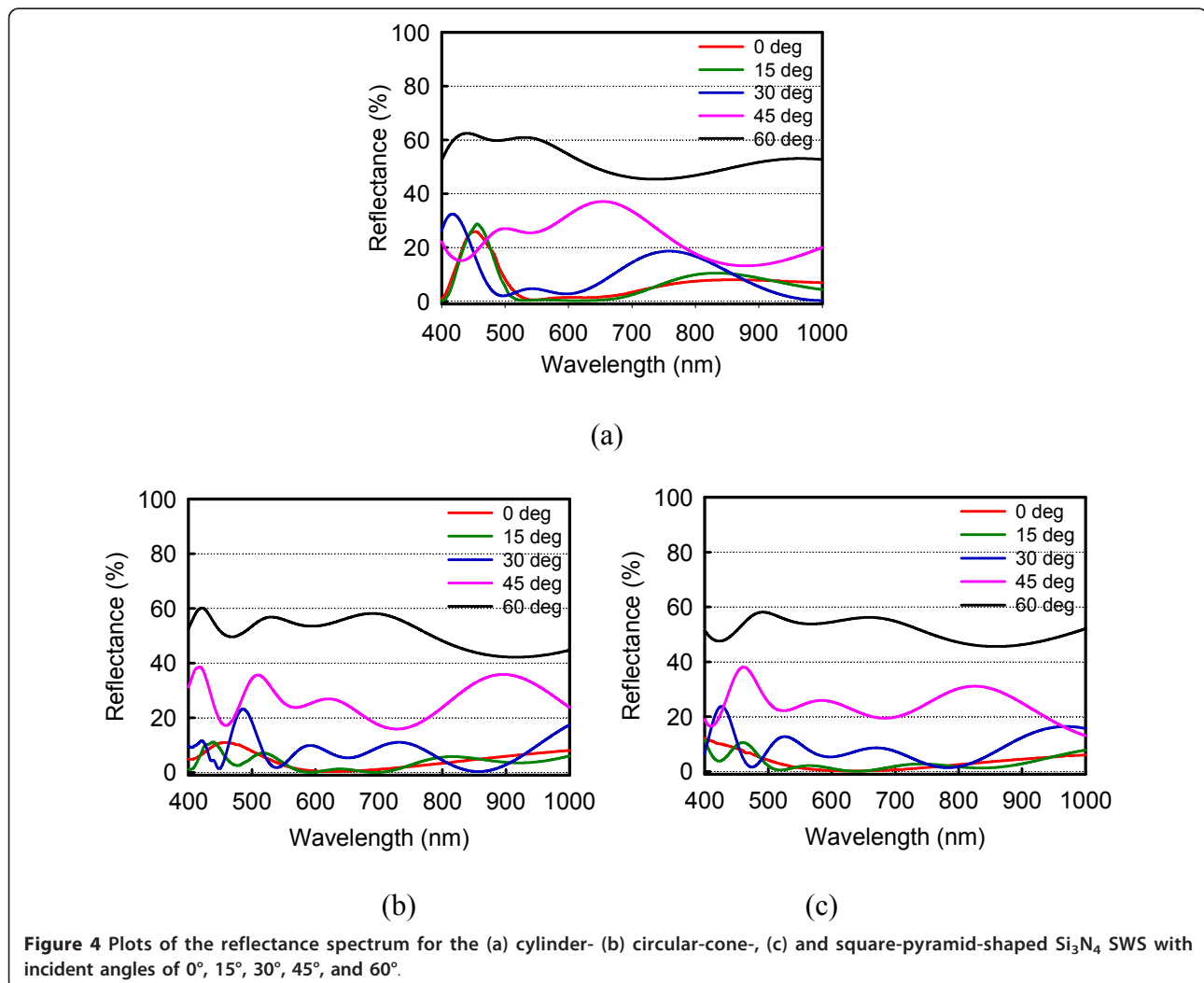


**Figure 2** Plot of the difference of reflectance spectrum of  $\text{Si}_3\text{N}_4$  SWS with the cylinder-, the right circular cone-, and the square pyramid-shaped structures as well as two different periodical configurations:  $1 \times 1$  (solid line) and  $2 \times 2$  arrays (dashed line) in the 3D FEM simulation.



occurs at wavelengths shorter than 600 nm. Based on this consequence, it is enable us to do simulation with more computational efficient using  $1 \times 1$  array of  $\text{Si}_3\text{N}_4$  SWS as a simulated unit cell with engineering acceptable accuracy. According to our recent RCWA work [4], the reflectance spectra are first plotted in Figure 3 using the optimal design parameters [1,4]. Also, the spectra calculated by a full 3D FE analysis with the same design parameters are indicated by dashed lines. For the cylinder-shaped  $\text{Si}_3\text{N}_4$  SWS, the reflectance spectra for RCWA and FE analysis are similar, but not agreed for the cone-shaped  $\text{Si}_3\text{N}_4$  SWS due to existing evanescent orders along the top of structures. This comparison confirms the importance of 3D FEM simulation which is beyond the RCWA approach [4].

Figure 4a-c shows the reflectance spectra with incident angles of  $0^\circ$ ,  $15^\circ$ ,  $30^\circ$ ,  $45^\circ$ , and  $60^\circ$  for the cylinder-, right circular cone-, and square pyramid-shaped  $\text{Si}_3\text{N}_4$  SWS, respectively. For the normal incidence case, the lowest



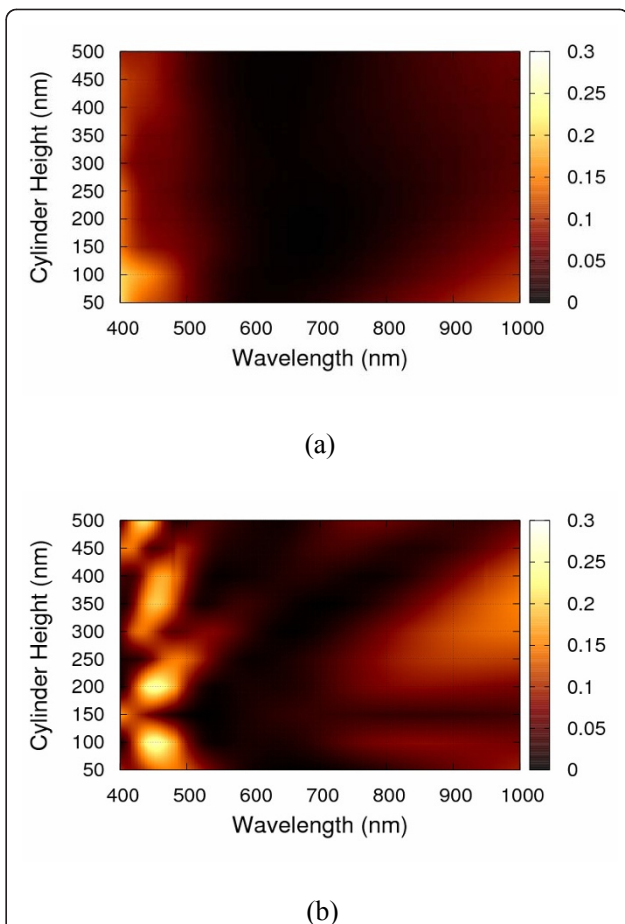
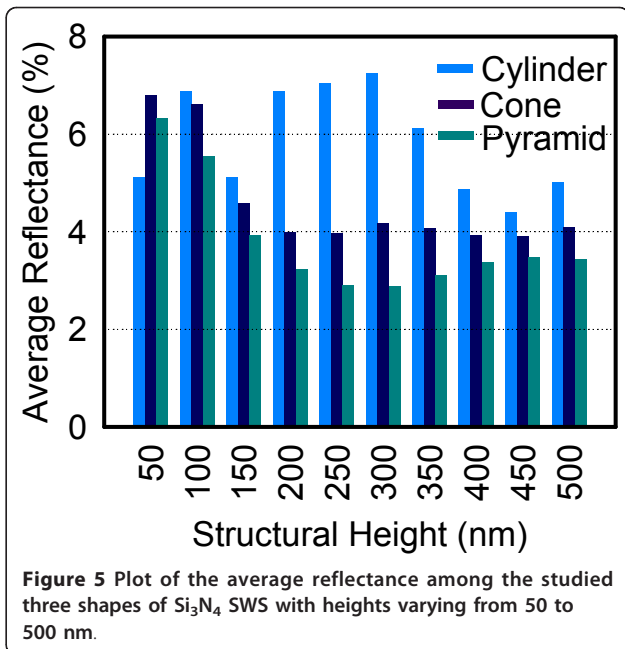
average reflectance among three structural shapes is 3.47% of square pyramid-shaped structure. The others are 6.86 and 4.42% for the cylinder- and the right circular cone-shaped  $\text{Si}_3\text{N}_4$  SWS, respectively. Meanwhile, as shown in Figure 4a-c, one can observe that the reflectance increases significantly with larger incident angles, resulting in average reflectance beyond 50%. Table 1 summarizes the average reflectance for various incident angles. Height effect on average reflectance of  $\text{Si}_3\text{N}_4$  SWS at normal incident angle with  $d = 130$  nm and  $s = 70$  nm is also calculated, as shown in Figure 5. The resulting average reflectance of pyramid-shaped  $\text{Si}_3\text{N}_4$  SWS nearly keeps lowest in comparison with the cylinder- and the right circular cone-shaped  $\text{Si}_3\text{N}_4$  SWS as the structural height is ranging from 50 to 500 nm. Figure 6 shows the reflectance dependence on the structural height and wavelength. The pyramid-shaped  $\text{Si}_3\text{N}_4$  SWS has lower reflectance and less sensitivity on structure height in comparison with the cylinder-shaped  $\text{Si}_3\text{N}_4$  SWS. Hence, the impact of process variation of structure height on solar cell performance is smaller for pyramid-shaped  $\text{Si}_3\text{N}_4$  SWS. Based on solar spectrum at the sea level revealed in American Society for Testing and Materials (ASTM) Standard Tables for Reference Solar Spectral Irradiances: Direct Normal and Hemispherical 37 Tilted Surface [9], we further estimate the reflected power density ( $\text{W}/\text{m}^2/\text{nm}$ ) defined by reflectance times incident power density, as shown in Figure 7. The higher reflected power density of cylinder-shaped  $\text{Si}_3\text{N}_4$  SWS (red line) indicates the less efficiency in the solar cell application. Therefore, normalized reflectance defined as

$$R_{\text{norm}} \equiv \frac{\text{Reflected power density}}{\text{Incident power density}} \quad (8)$$

reveals the real power efficiency applied in the solar cell application. Figure 8 shows the normalized reflectance for the cylinder-, right circular cone-, and square pyramid-shaped  $\text{Si}_3\text{N}_4$  SWS, respectively. The square pyramid-shaped  $\text{Si}_3\text{N}_4$  SWS again shows the lowest normalized reflectance 3.13% while the cylinder- and the right circular cone-shaped  $\text{Si}_3\text{N}_4$  SWSs have 6.66 and 4.12%, respectively.

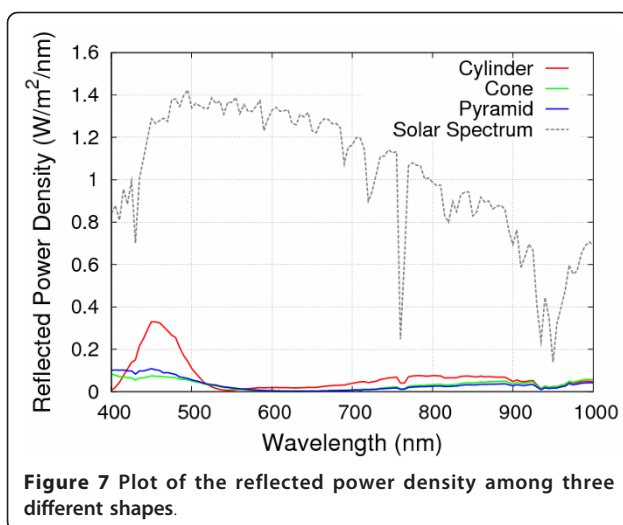
**Table 1 Summary of the average reflectance of  $\text{Si}_3\text{N}_4$  SWS with various incident angles**

Average reflectance (%)	0°	15°	30°	45°	60°
Cylinder shape	6.86	6.70	9.95	23.13	52.78
Circular cone shape	4.42	3.64	7.79	26.68	50.98
Square pyramid shape	3.47	3.15	8.88	24.40	51.44



**Figure 6** 3D view for the height effect on the reflectance with respect to different wavelength. **(a)** The pyramid-shaped  $\text{Si}_3\text{N}_4$  SWS has lower reflectance and less sensitivity on structure height in comparison with **(b)** the cylinder-shaped  $\text{Si}_3\text{N}_4$  SWS.





#### 4. Conclusions

In this study, the reflective property of unit cell with a validated Floquet boundary condition has been calculated using a full 3D FE simulation. Considering various incidence angles and height effect on three experimentally observed structural shapes of  $\text{Si}_3\text{N}_4$  SWS, we have concluded that the pyramid-shaped  $\text{Si}_3\text{N}_4$  SWS has best reflective property in the analysis of morphological effect. Compared with the results of RCWA, the reflective property calculated by the full 3D FEM is significantly deviated from the results from RCWA, giving the hint that a detailed and comprehensive methodology is dispensable for the design of  $\text{Si}_3\text{N}_4$  SWS. The results of computed reflectance, reflected power density, and normalized reflectance have shown that the pyramid shape of SWS may have the best reflectance property in the optical region from 400 to 1000 nm which is useful for silicon solar cell applications. The optimized pyramid-

shaped  $\text{Si}_3\text{N}_4$  SWS is currently under plan for implementation with silicon solar cells.

#### Abbreviations

3D: three-dimensional; ARC: antireflection coating; FEM: finite element method; RCWA: rigorous coupled-wave analysis;  $\text{Si}_3\text{N}_4$ : silicon nitride; SLAR: single layer; SWS: subwavelength structure.

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#### Authors' contributions

M-YL, H-WC, and Z-LL performed the numerical simulation and data analysis, YL conducted whole study including manuscript preparation. All the authors read and approved the final manuscript.

#### Competing interests

The authors declare that they have no competing interests.

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